**VOC aggregation in EURODELTA-TREND models**

# CHIMERE

VOC = sum of C2H6 C2H6 NC4H10 NC4H10 NC4H10 NC4H10 C2H4 C2H4 C3H6 C3H6 C3H6 OXYL OXYL OXYL OXYL OXYL OXYL OXYL OXYL C5H8 C5H8 C5H8 C5H8 C5H8 APINEN APINEN APINEN APINEN APINEN APINEN APINEN APINEN APINEN APINEN in µgC/m3

# CMAQB

VOCs deliveries for CMAQB are in ppm (raw units in the model) and they

are the sum of lumped species in the chemical mechanism CB05

(http://www.camx.com/files/cb05\_final\_report\_120805.aspx) as follows:

VOC=FORM+ALD2+C2O3+PAN+NTR+FACD+AACD+PACD+PAR+ETH+OLE+ISOP+ISPD+TERP+TOL+XYL+CRES+ROR+MGLY+MEOH+ETOH+ETHA+IOLE+ALDX+PANX+MEPX+ROOH+BENZENE+SESQ

# EMEP

VOC provided in µg/m3

Aggregation

NMVOC\_GROUP = (/ PAN,MPAN,CH3COO2,MACR,GLYOX,MGLYOX,MAL,MEK,MVK,HCHO,CH3CHO,C2H6,NC4H10,C2H4,C3H6,OXYL,C5H8,APINENE,CH3O2H,C2H5OOH,BURO2H,ETRO2H,PRRO2H,MEKO2H,MALO2H,MACROOH,MACO3H,MACO2H,CH3COO2H,CH3OH,C2H5OH,ACETOL,GAS\_ASOA\_OC,PART\_ASOA\_OC,GAS\_BSOA\_OC,PART\_BSOA\_OC,PART\_FFUELOA25\_OC,PART\_WOODOA25\_OC,PART\_FFIREOA25\_OC,PART\_OC10,PART\_OC25,NONVOL\_FFUELOC25,NONV\_FFUELOC\_COARSE,NONVOL\_WOODOC25,NONVOL\_BGNDOC,NONVOL\_FFIREOC25,POM\_F\_WOOD,POM\_F\_FFUEL,POM\_C\_FFUEL,EC\_F\_WOOD\_NEW,EC\_F\_WOOD\_AGE,EC\_C\_WOOD,EC\_F\_FFUEL\_NEW,EC\_F\_FFUEL\_AGE,EC\_C\_FFUEL,FFIRE\_OM,FFIRE\_BC,ASOC\_NG100,ASOC\_UG1,ASOC\_UG10,ASOC\_UG1E2,ASOC\_UG1E3,BSOC\_NG100,BSOC\_UG1,BSOC\_UG10,BSOC\_UG1E2,BSOC\_UG1E3,FFFUEL\_NG10,WOODOA\_NG10,FFIREOA\_NG10 /)

Emission split:

# VOC splits for EmChem09

# Produced by Garry Hayman from NAEI2000\_09Nov 2009

# Key-word, MASS\_ASSUMED= 0 by default,

# change when emissions have artificial mass, e.g. 46 for NOx as NO2

: MASS\_ASSUMED 0

99 99 C2H6 NC4H10 C2H4 C3H6 C5H8 OXYL CH3OH C2H5OH HCHO CH3CHO MEK GLYOX MGLYOX UNREAC #HEADERS

#DATA

0 1 12.559 14.836 2.406 4.376 0.000 9.479 0.000 0.000 55.691 0.034 0.620 0.000 0.000 -0.000

0 2 12.589 39.790 8.174 10.767 0.000 18.632 0.000 3.912 5.586 0.207 0.089 0.000 0.000 0.255

0 3 4.996 35.610 9.044 2.089 0.000 18.323 0.561 3.034 24.134 0.059 1.347 0.000 0.000 0.805

0 4 2.652 34.519 5.458 4.257 0.142 13.380 1.176 31.414 0.077 0.978 1.608 0.000 0.000 4.337

0 5 17.842 79.895 0.018 1.569 0.008 0.505 0.000 0.000 0.078 0.000 0.000 0.000 0.000 0.085

0 6 0.444 44.052 0.244 0.678 0.008 17.904 6.101 16.416 0.011 0.000 9.965 0.000 0.000 4.176

0 7 4.832 36.698 6.796 10.896 0.000 35.051 0.000 0.000 2.700 2.606 0.421 0.000 0.000 0.000

0 8 3.775 47.416 6.636 10.608 0.000 24.676 0.000 0.000 3.115 3.261 0.235 0.146 0.117 0.014

0 9 25.718 36.778 5.237 1.830 1.153 7.881 0.427 2.439 16.060 0.000 0.093 0.000 0.000 2.383

0 10 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 100.000

0 11 0.000 0.000 0.000 0.000 100.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000

# LOTO

VOC provided in µg/m3

Aggregation

VOC= "form\* 1.04\*dens +ald\* 1.49\*dens +mgly\* 2.49\*dens +par\* 0.52\*dens +ole\* 0.93\*dens +eth\* 0.97\*dens +tol\* 3.18\*dens +cres\* 3.73\*dens +xyl\* 3.67\*dens +iso\* 2.35\*dens +terp\* 4.70\*dens" ;

Emission split

VOC split:

BEGIN VOC profiles CBM4

UNIT [mol/kg VOC]

code category\_name OLE PAR TOL XYL FORM ALD KET ACET ETH UNR

1 "Power\_generation" 0.208 29.30 0.718 0.626 3.506 0.358 0.000 0.000 0.106 5.206

2 "Non-industrial combustion" 1.869 19.77 0.317 0.083 1.766 1.362 0.000 0.000 4.840 10.65

3 "Industrial\_combustion" 0.808 26.89 0.942 1.030 2.566 0.888 0.000 0.000 1.099 5.930

4 "Industrial\_processes" 0.991 38.92 0.307 0.152 1.464 0.075 0.000 0.000 2.048 10.77

5 "Fossil fuel production and distribution" 0.345 40.17 0.041 0.018 0.077 0.562 0.000 0.000 0.064 20.04

6 "Solvent\_use" 0.207 40.10 0.920 0.721 0.000 0.577 0.000 0.000 0.000 3.590

7 "Road transport" 1.557 29.26 1.505 1.741 1.352 0.995 0.000 0.000 2.573 5.638

8 "Non-road transport" 1.131 30.49 0.235 1.287 2.494 1.145 0.000 0.000 4.536 5.006

9 "Waste" 0.529 13.39 0.208 0.172 0.457 0.430 0.000 0.000 1.176 3.568

10 "Agriculture" 2.126 21.19 0.366 0.090 1.953 1.665 0.000 0.000 4.504 10.67

END VOC profiles CBM4

# MINNI

VOC in µg/m3

Sum of

ROOH PAN PAN2 HCHO CCHO RCHO MEK RNO3 MGLY ETHE OLE1 OLE2 ISOP TRP1 ALK1

ALK2 ALK3 ALK4 ALK5 ARO1 ARO2 HC2H CO2H C6H6 ACET PRD2 GLY PHEN CRES BALD NPHE PBZN MEOH METH MVK ISPD MA\_PAN CO3H RC3H RC2H COOH BACL

# POLR

POLR VOC outputs are in µg/m3, and they are the sum of CB05 lumped

species. The VOC ouput is the sum of the aggregated species.

Aggregation matrix

POLR\_aggregation\_cb05-siream.dat

VOC split

POLR\_Spe-NMVOC.dat

# WRFC

My VOC deliveries were in ug/m3 -- so including all the hydrogens and oxygens. Unfortunately, I don't have all the raw output still, but for the 2010 base run I could provide the total in ug Carbon/m3 as well as the distribution of modeled concentrations of individual VOC species.

I also have a distribution of emitted VOCs (by SNAP), if you are interested in that.